

Spin Splitting in Quantum Wires with Perturbed Axial Symmetry

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We investigate theoretically perturbations to the confining potential capable of lifting spin degeneracy in axially symmetric quasi-one-dimensional electron gases with the spin-orbit interaction. The role of two different types of perturbations breaking axial symmetry of the system: of non-electromagnetic and electromagnetic origin is analyzed. We found that these two types of perturbations have a fundamental distinction in their effects on energy spectra. The influence of the scale of perturbation upon the value of spin splitting is investigated and it is shown that under certain conditions such splittings can be observed in the experiment.

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I. INTRODUCTION

Spin splitting in energy bands of quasi-one-dimensional and two-dimensional electron gases (Q1DEG's and 2DEG's, respectively) in zero magnetic field has been studied extensively both theoretically^{1,2,3,4,9} and experimentally^{10,11,12,13,14} over the two past decades. Such an interest was partially produced by the prospect of creating new electronic devices which exploit spin-polarized transport^{15,16}. The appearance of spin splitting in energy spectra of realistic heterostructures, which are usually described by Q1DEG's and 2DEG's models, was ascribed mainly to Rashba¹⁷ and Dresselhaus¹⁸ terms in the corresponding Hamiltonians. Such Hamiltonians usually possess two distinctive features: (i) as parameters varied in theoretical constructs they contain merely coefficients placed before splitting-inducing terms in order to achieve an agreement with the experiment⁴ and (ii) they include confining potentials for effective reduction of the dimensions of the system. While a thorough analysis of the effect of different splitting-inducing terms upon energy spectra has been carried out and their role understood, the choice of confining potentials is still limited mainly to simple (and model) hard-wall⁵ and parabolic^{6,7,8,9} ones. Such a choice is conditioned by the fact that the corresponding non-perturbed problems are often explicitly solvable. At the same time this may give rather simplified picture of real energy band structure of the model systems. The common step to avoid this shortcoming is to change the form of a potential slightly, for example, by accounting for non-parabolicity terms. Here, however, we do not touch upon this and related issues which are unlikely to seriously influence the general spectral picture, but introduce confining potentials which are themselves capable of giving rise to spin splitting beyond Rashba and Dresselhaus mechanisms.

In this paper we investigate an infinite Q1DEG produced out of 3-dimensional system by means of a 2-dimensional confining potential. The initial confining potential is assumed to be axially symmetrical and have the electromagnetic nature. Axially symmetrical quan-

tum wires are rather easy to investigate theoretically and, what is more important, they are not just a theoretical model, but may be prepared practically (see, for instance¹⁹, and references therein). We also neglect Coulomb interaction between electrons, which is quite realistic given that it can be accounted for by the renormalization of the SO coupling constant²⁰. Spin-orbit (SO) interaction emanates from the Pauli equation and is of the form:

$$\frac{e\hbar}{4m_e^2c^2}\vec{\nabla}\varphi\cdot(\vec{\sigma}\times\hat{p}), \quad (1.1)$$

where m_e is the effective electron mass, φ is the scalar electromagnetic potential, $\vec{\sigma}$ is the Pauli matrices vector, and \hat{p} is the momentum operator. The vector electromagnetic potential \vec{A} is put equal to zero in all the systems this paper deals with.

The described system possesses a spectrum in which every energy level is twice degenerate. We introduce a perturbation (not necessarily small) to the confining potential that breaks axial symmetry of the system. This leads to lifting spin degeneracy, the mechanism of which being different depending on whether the perturbation has electromagnetic or non-electromagnetic origin. The investigation of effects, which such perturbations have on spectra, is yet more important if one takes into account that perturbations conditioning deviations from axial symmetry are always present in the experiment. We show that under certain conditions the spin splitting, originated by potentials in question, may be large enough to be detected.

II. AXIALLY SYMMETRIC CONFINING POTENTIAL

Let us first consider the case of axially symmetric confining potential created by purely electrostatic field. The inclusion of SO interaction into the Hamiltonian significantly hinders seeking the solution of the corresponding

eigenvalue problem, so that one may expect to find solutions only by means of perturbation theory or numerical calculations. That is why we chose a parabolic confining potential

$$\hat{V}_{conf} = \frac{m_e \omega^2}{2} \rho^2, \quad (2.1)$$

where ω has the dimension of frequency and measures the strength of the potential and ρ is the lateral cylindrical coordinate. This potential will provide us with a convenient zero approximation to the solution. The Hamiltonian of our problem has the following form:

$$\hat{H} = \frac{\hat{p}^2}{2m_e} + \hat{V}_{conf} + \mu \hat{V}_{SO} + \frac{\hbar^2 \omega^2}{4m_e c^2}. \quad (2.2)$$

Here the SO interaction is

$$\hat{V}_{SO} = -\frac{i\hbar^2 \omega^2}{4m_e c^2} \left[-i\sigma_z \frac{\partial}{\partial \theta} + \rho \begin{pmatrix} 0 & -ie^{-i\theta} \\ ie^{i\theta} & 0 \end{pmatrix} \frac{\partial}{\partial z} \right]. \quad (2.3)$$

The positive constant μ defines the strength of the SO interaction. At $\mu = 1$ the Hamiltonian (3) naturally stems from the usual Pauli Hamiltonian

$$\begin{aligned} \hat{H}_P = & \frac{\hat{p}^2}{2m_e} + e\varphi - \frac{\hat{p}^4}{8m_e^3 c^2} \\ & - \frac{e\hbar}{4m_e^2 c^2} \vec{\sigma} \cdot (\vec{E} \times \hat{p}) - \frac{e\hbar^2}{8m_e^2 c^2} \text{div} \vec{E} \end{aligned} \quad (2.4)$$

if one puts the scalar potential φ equal to $m_e \omega^2 \rho^2 / 2e$ and neglects the term $\hat{p}^4 / 8m_e^3 c^2$, which does not influence the spin-splitting.

The solution to the zero approximation eigenvalue problem

$$\left(\frac{\hat{p}^2}{2m_e} + \hat{V}_{conf} \right) \chi \equiv \hat{H}_0 \chi = E \chi \quad (2.5)$$

was found in 1928 by Fock²¹. It reads

$$\chi_{nlk_z}(\rho, z, \theta) = \Psi_{nl}(\rho) Y_l(\theta) R_{k_z}(z), \quad (2.6)$$

$$\begin{aligned} \Psi_{nl}(\rho) = & \sqrt{\frac{2n!}{(n+|l|)!}} \frac{1}{\rho_\omega} \exp\left[-\frac{1}{2} \left(\frac{\rho}{\rho_\omega}\right)^2\right] \left(\frac{\rho}{\rho_\omega}\right)^{|l|} \\ & \times L_n^{|l|} \left(\frac{\rho^2}{\rho_\omega^2}\right), n = 0, 1, 2, \dots, l = 0, \pm 1, \pm 2, \dots, \end{aligned} \quad (2.7)$$

$$Y_l(\theta) = \frac{1}{\sqrt{2\pi}} e^{il\theta}, \quad R_{k_z}(z) = \frac{1}{\sqrt{V}} e^{ik_z z}.$$

The radial functions $\Psi_{nl}(\rho)$ comprise the generalized Laguerre polynomials $L_n^{|l|}$. The value $\rho_\omega = \sqrt{\hbar/m_e \omega}$ serves as a characteristic scale in our problem. The function $R_{k_z}(z)$ corresponds to a plane wave with k_z being the longitudinal wave number and normalization is based on the property $\delta(0)/V \rightarrow 1$ as $V \rightarrow \infty$. The functions (2.6) form a complete orthonormal set. The energy corresponding to the state χ_{nlk_z} is given by

$$E_{nlk_z}^{(0)} = \hbar\omega(2n + |l| + 1) + \frac{\hbar^2 k_z^2}{2m_e}. \quad (2.8)$$

It is important that the whole energy may be separated into two conserving constituents: the lateral and longitudinal ones, and the lateral spectrum is equidistant. This property holds true as long as Hamiltonian depends on z only by the way of derivatives $\partial^n / \partial z^n$. The longitudinal component of the wave vector, k_z , remains constant during the motion and is convenient to be considered as a parameter. At a given k_z the eigenfunctions (2.6) form a complete set in the corresponding subspace and may be chosen as a basis for seeking the approximate solutions of the eigenvalue problem

$$\hat{H}\Phi = E\Phi. \quad (2.9)$$

The Hamiltonian (2.2) has a 2×2 -matrix structure, so its basis eigenfunctions must be of a two-component vector form. Such two-component functions form the fundamental system of the matrix Hamiltonian

$$\begin{pmatrix} \hat{H}_0 & 0 \\ 0 & \hat{H}_0 \end{pmatrix} \quad (2.10)$$

and read:

$$\chi_{\uparrow, nlk_z} = \begin{pmatrix} \chi_{nlk_z} \\ 0 \end{pmatrix}, \quad \chi_{\downarrow, nlk_z} = \begin{pmatrix} 0 \\ \chi_{nlk_z} \end{pmatrix}. \quad (2.11)$$

The diagonal $\langle \chi_{(\uparrow, \downarrow), nlk_z} | V_{SO} | \chi_{(\uparrow, \downarrow), mkk_z} \rangle$ and off-diagonal $\langle \chi_{(\uparrow, \downarrow), nlk_z} | V_{SO} | \chi_{(\downarrow, \uparrow), mkk_z} \rangle$ matrix elements as well as matrix elements which appear in Section III may be easily calculated. The convolutions of two-component vectors with 2×2 matrices were performed according to the usual matrix multiplication rules. The integrals needed to be taken in order to calculate the matrix elements may be written as a product of three integrals over ρ , θ and z . The integrals over ρ were taken according to the formula²⁴:

$$\int_0^\infty x^\alpha \rho_\omega^2 \chi_{mk}(x) \chi_{nl}(x) dx = \frac{\Gamma(1+\alpha+(l+k)/2)}{\sqrt{m!n!(m+|k|)!(n+|l|)!}} \frac{\Gamma(1+n+l)}{\Gamma(1+l)} \frac{\Gamma((k-l)/2-\alpha+m)}{\Gamma(2+(l-k)/2+\alpha)} \times$$

$${}_3F_2[-n, 2+\alpha+(l+k)/2, 2+\alpha+(k-l)/2; 1+k, 2+\alpha-m+(k-l)/2; 1]. \quad (2.12)$$

In concordance with the normalization rules for $Y_l(\theta)$ ²² the integrals over θ and z are simple Fourier transformations. For instance, what follows is a typical integral one meets in the calculation of the matrix elements from Section III:

$$\int_0^{2\pi} \cos^2\left(\frac{N\theta}{2}\right) e^{i(k-l)\theta} d\theta = \frac{\pi}{2} (2\delta_{k,l} + \delta_{k-l,N} + \delta_{k-l,-N}). \quad (2.13)$$

In numerical calculations throughout this paper we used 30 up- and 30 down-basis functions. This allowed

us to obtain 60 energy levels with a difference from the exact values only in the 9th significant digit. The value of ω was chosen to be 10^{15} sec^{-1} and m_e^* was put equal to $0.05m_e$.

The Fig. 1 shows several first lateral energy levels of the Hamiltonians \hat{H}_0 and \hat{H} . The lateral energies pertaining to \hat{H}_0 are degenerate with the multiplicity $2(2n+|l|+1)$. Thus, every q -th eigenvalue (counting from the bottom of the quantum well) of \hat{H}_0 is $2q$ times degenerate and splits into q branches in transition to \hat{H} . Therefore, \hat{V}_{SO} leaves 2-fold spin degeneracy of every energy level.

III. PERTURBED AXIALLY SYMMETRIC CONFINING POTENTIAL

A. Non-electromagnetic perturbation

The perturbation we will deal with here and in the subsequent part of this section is

$$\hat{V}_{pert} = A \frac{m_e \omega^2}{2} \rho^2 \cos^2\left(\frac{N\theta}{2}\right), \quad (3.1)$$

$$A \geq 0, \quad N \in 0, 1, 2, \dots \quad (3.2)$$

The dimensionless constant parameters A and N define the amplitude and the number of ‘lobes’ of the perturbation, respectively (see Fig. 2). At $N = 2$ our problem resembles the 2D type of the problem solved by Migdal²³. In this part we investigate the effect which \hat{V}_{pert} has on the spectrum considering it to be of non-electromagnetic nature (\hat{V}_{pert}^{n-el}). Under the non-electromagnetic nature of the perturbation we imply that it does not affect φ and \vec{E} in the Hamiltonian (2.4), but is simply added to the right-hand side of (2.4). On the other hand, the electromagnetic perturbation \hat{V}_{pert}^{el} , which is regarded in the next subsection, does influence φ and \vec{E} .

The case of the non-electromagnetic perturbation is especially interesting because at even N \hat{V}_{pert}^{n-el} leaves the inversion symmetry ($\theta \rightarrow \theta + \pi, z \rightarrow -z$) of the Hamiltonian intact, although breaks its axial symmetry. This should have a non-trivial effect on the spin splitting in the energy spectra. The increased (in comparison with the free space value $\mu = 1$) value of μ , equal to 10^3 , approximately corresponds to that of the constant β from the work⁹ and may not only allow to draw correlations

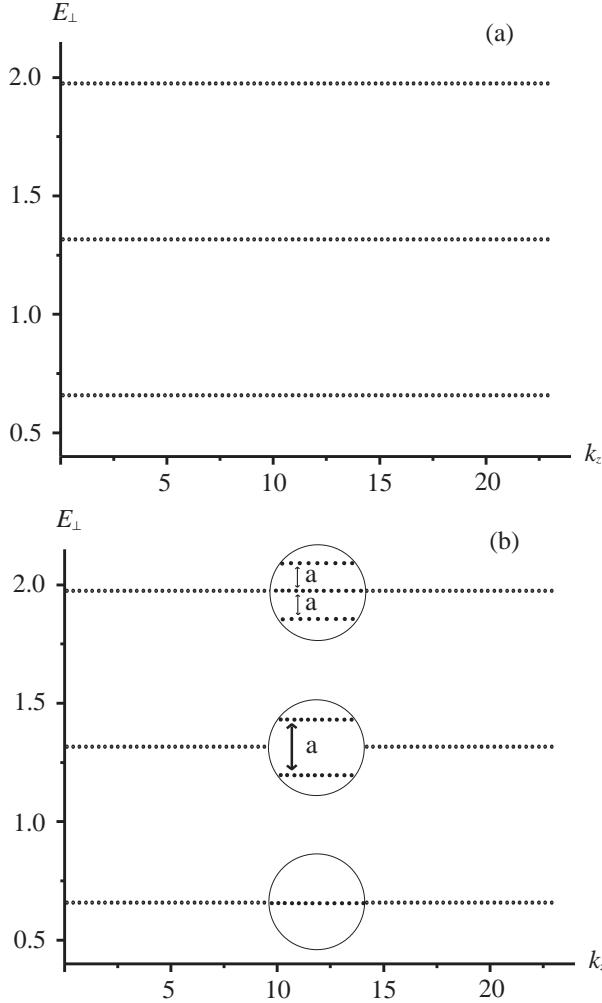


FIG. 1: (a) The spectrum of \hat{H}_0 ; (b) the spectrum of \hat{H} , $\mu = 1$. Energy E is measured in eV, k_z is measured in units of 10^6 cm^{-1} , $a = 8.47 \cdot 10^{-6} \text{ eV}$.

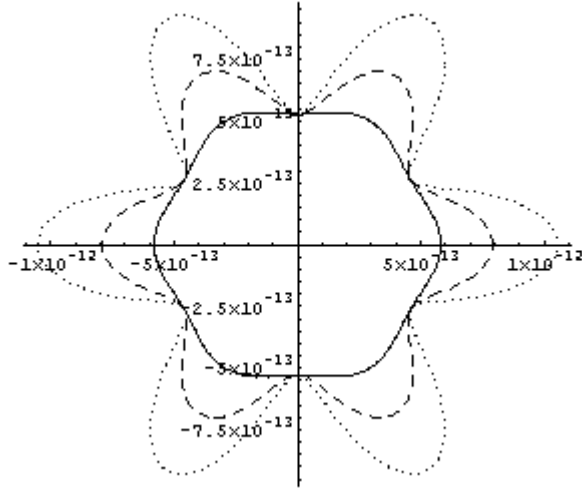


FIG. 2: The polar plot of the potential $\hat{V}_{conf} + \hat{V}_{pert}$, $N = 6$, $\rho = \rho_\omega$: dotted line – $A = 1.0$, dashed line – $A = 0.5$, solid line – $A = 0.1$.

with the results of the latter, but can also help to elucidate the role of SO interaction in the formation of energy band structure. The Fig. 3 demonstrates spin splitting for various values of the parameters N , A , and μ . At even values of N no spin splitting is predicted for any energy level. This may be explained by higher symmetry of the potential in this case. At odd N the spin splitting follows a rather peculiar pattern: with the growth of N the number of non-perturbed energy level (if the ground state has number zero) at which spin splitting occurs for the first time enhances. The Table 1 illustrates this behavior.

Table 1. Energy levels of the Hamiltonian H which undergo splitting in the case of non-electromagnetic perturbation \hat{V}_{pert}^{n-el} . The ground state has number zero.

| N | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
|--------------|-----|------|-----------|------|---------|------|----------|
| Level number | all | none | 2,3,9,... | none | 4,6,... | none | 7,10,... |

Very important for practical reasons is the question of how spin splitting depends on the amplitude of perturbation A . The Table 2 shows that the magnitude of spin splitting decreases very rapidly as A gets smaller, so that minute perturbations give almost indiscernible splitting. The rise of the contribution of SO interaction (the increase of μ) does not lead to any fundamental changes in the energy spectra, but increases almost proportionally to μ the values of spin splitting. For example, at $A = 1$, $N = 3$, $\mu = 10^3$ and $k_z = 2 \cdot 10^7 \text{ cm}^{-1}$ spin splittings $|\Delta_d|$, where d is the number of the unperturbed energy level, for $d = 2$ and $d = 3$ are $2.32 \cdot 10^{-2} \text{ eV}$ and $3.07 \cdot 10^{-2} \text{ eV}$, respectively.

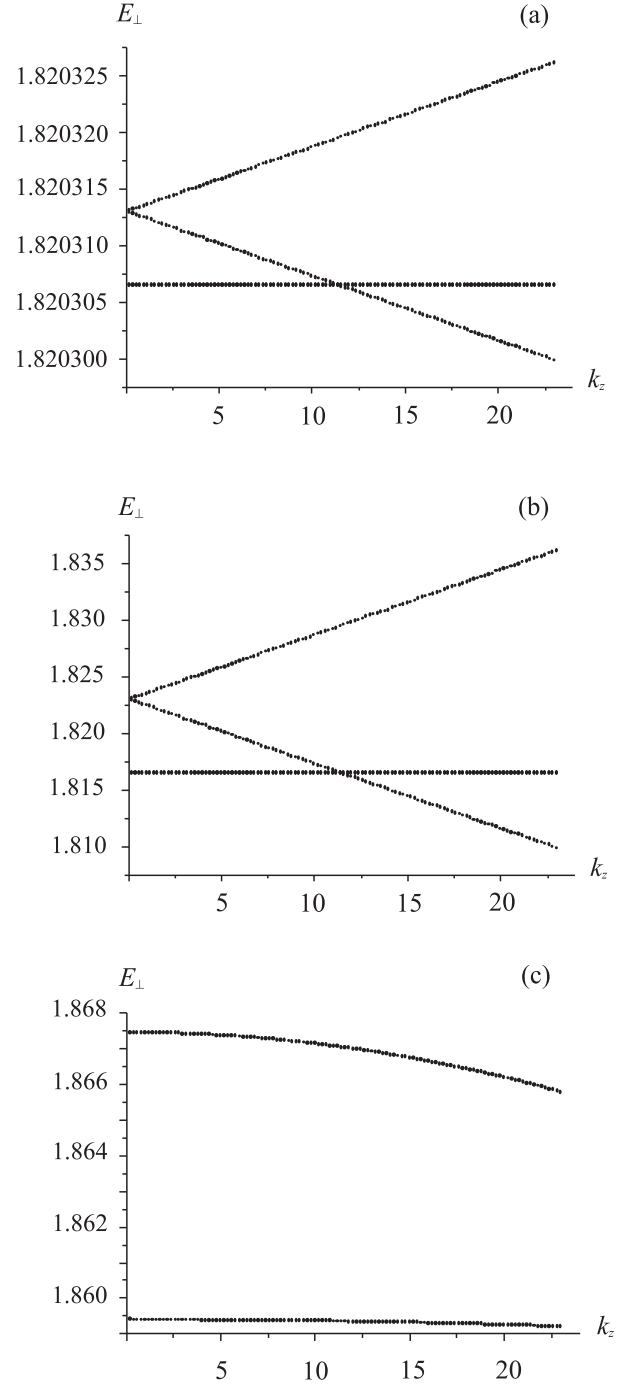


FIG. 3: The spin splitting originated by non-electromagnetic perturbation \hat{V}_{pert}^{n-el} . Energy E is measured in eV, k_z is measured in units of 10^6 cm^{-1} . (a) $A = 1$, $\mu = 1$, $N = 3$, $d = 1, 2$; (b) $A = 1$, $\mu = 10^3$, $N = 3$, $d = 1, 2$; (c) $A = 1$, $\mu = 10^3$, $N = 4$, $d = 1, 2$.

B. Electromagnetic perturbation

Treated as being of electromagnetic nature, the perturbation \hat{V}_{pert}^{el} , which formally has the form (3.1), results

in the following Hamiltonian:

$$\hat{H}' = \hat{H} + \Delta\hat{H}. \quad (3.3)$$

Here

$$\begin{aligned} \Delta\hat{H} = & -\frac{i\hbar^2\omega^2}{4m_e c^2} \left\{ A\rho \cos^2\left(\frac{N\theta}{2}\right) \begin{pmatrix} 0 & -ie^{-i\theta} \\ ie^{i\theta} & 0 \end{pmatrix} \frac{\partial}{\partial z} + A\frac{\hbar^2\omega^2}{8m_e c^2} \left[1 - \left(\frac{N^2}{4} - 1\right) \cos(N\theta) \right] + \right. \\ & \left. \frac{AN}{2}\rho \cos\left(\frac{N\theta}{2}\right) \sin\left(\frac{N\theta}{2}\right) \begin{pmatrix} 0 & e^{-i\theta} \\ e^{i\theta} & 0 \end{pmatrix} \frac{\partial}{\partial z} - \frac{AN}{2}\rho \cos\left(\frac{N\theta}{2}\right) \sin\left(\frac{N\theta}{2}\right) \sigma_z \frac{\partial}{\partial \rho} - A \cos^2\left(\frac{N\theta}{2}\right) \sigma_z \frac{\partial}{\partial \theta} \right\}. \end{aligned} \quad (3.4)$$

The matrix elements of $\Delta\hat{H}$ in space of the functions (2.13) can also be explicitly calculated (see Eqns. (2.13)-(2.15)). The Fig. 4 demonstrates the spin splitting originated by \hat{V}_{pert}^{el} . Now all the energy levels are non-degenerate for both even and odd values of N . The magnitude of spin splitting goes down with the decrease of A approximately with the same rate as it does in the case of non-electromagnetic perturbation (see Table 2). It is clear from the Table 2 that as A decreases, the difference between non-electromagnetic and electromagnetic cases gradually vanishes.

Table 2. The value of spin splitting Δ_d (eV) at various amplitudes A of the perturbation \hat{V}_{pert} . $N = 3$, $\mu = 1$, $k_z = 2 \cdot 10^7 \text{ cm}^{-1}$.

| A | | 1 | 10^{-1} | 10^{-2} | 10^{-3} |
|------------------------------------|--|----------------------|----------------------|----------------------|----------------------|
| $\hat{V}_{pert}^{n-el} \Delta_2 $ | | $2.29 \cdot 10^{-5}$ | $4.16 \cdot 10^{-6}$ | $4.06 \cdot 10^{-7}$ | $4.05 \cdot 10^{-8}$ |
| $\hat{V}_{pert}^{n-el} \Delta_3 $ | | $3.04 \cdot 10^{-5}$ | $6.16 \cdot 10^{-6}$ | $6.09 \cdot 10^{-7}$ | $6.07 \cdot 10^{-8}$ |
| $\hat{V}_{pert}^{el} \Delta_2 $ | | $9.63 \cdot 10^{-6}$ | $2.87 \cdot 10^{-6}$ | $4.04 \cdot 10^{-7}$ | $4.05 \cdot 10^{-8}$ |
| $\hat{V}_{pert}^{el} \Delta_3 $ | | $1.75 \cdot 10^{-5}$ | $4.65 \cdot 10^{-6}$ | $6.08 \cdot 10^{-7}$ | $6.07 \cdot 10^{-8}$ |

IV. CONCLUSION

In this work we studied theoretically a 3D gas of non-interacting electrons which was transformed into a Q1DEG by means of 2D confining potential. We have solved the Pauli equation numerically for this system with perturbed axially-symmetric, parabolic confining potential. The non-perturbed axially symmetric potential \hat{V}_{conf} was assumed to be created by electromagnetic field with the scalar potential $\varphi = m_e \omega^2 \rho^2 / 2e$. Two different types of perturbations capable of lifting the spin degeneracy are considered: of electromagnetic and non-electromagnetic nature. We have found that these two types of perturbation have different effects on the energy spectra. While the electromagnetic perturbation splits

all the levels, the non-electromagnetic one in most cases (besides the case with $N = 1$) leaves the spin degeneracy of some levels. We have found that for large perturbations ($A = 1$) the value of spin splitting is large enough to be detected in the experiment (10^{-5} eV and higher).

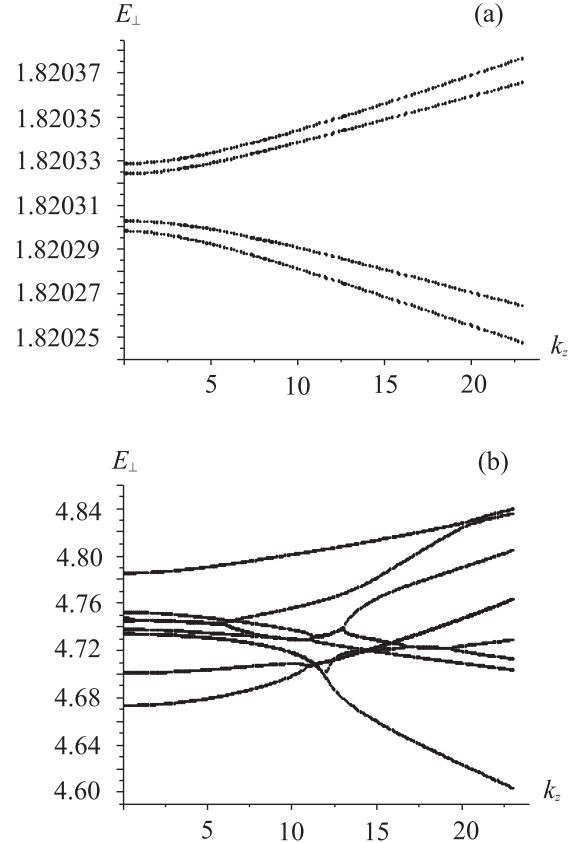


FIG. 4: The spin splitting originated by electromagnetic perturbation \hat{V}_{pert}^{el} . Energy E is measured in eV, k_z is measured in units of 10^6 cm^{-1} . (a) $A = 1$, $\mu = 1$, $N = 3$, $d = 1, 2$; (b) more complex behavior of high-lying levels, $A = 1$, $\mu = 10^3$, $N = 4$, $d = 21, \dots, 25$.

As A decreases, spin splitting also goes down linearly or even faster. Therefore, if practically created axially-symmetric potentials only slightly deviate from the axial symmetry, spin splitting originated by discussed in this work mechanism is unlikely to be observed. However, if a confining potential possesses only rough axial symmetry, the additional splitting of the energy levels may appear.

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